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CONFIDENCE REGIONS FOR VARIANCE COMPONENTS

IN UNBALANCED MIXED LINEAR MODELS

by

Alan P. Fenech and David A. Harville[1]
University of California-Davis and Iowa State University

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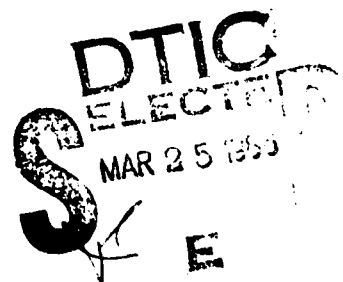
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ABSTRACT

We present a general procedure for obtaining exact confidence

regions for the variance components in unbalanced mixed linear models.

The procedure utilizes, as pivotal quantities, quadratic forms that may

depend on the variance components in a complicated way and that are dis-

tributed independently as chi-square variates. In the special case of

balanced classificatory models, the pivotal quantities simplify to scalar

multiples of sums of squares from the usual analysis of variance. The

procedure can be easily modified so as to obtain an exact confidence

region for ratios of variance components and can be regarded as a

generalization of Wald's procedure for obtaining a confidence interval

for a single variance ratio.

1. INTRODUCTION

Suppose that y is an n x 1 observable vector that follows the general mixed linear model

$$(1.1) \qquad y = X_0\beta_0 + X_1 b_1 + \ldots + X_k b_k + b_{k+1}$$

where X_i is an n x m_i known matrix (i = 0,...,k), and β_0 is an m_0 x 1 vector of unknown parameters, b_i is an m_i x 1 unobservable random vector whose distribution is $N(0, \sigma_i^2 I)$, that is, multivariate normal with mean vector 0 and variance-covariance matrix $\sigma_i^2 I$ (i=1,...,k+1), and σ_1^2, ...,σ_{k+1}^2 are unknown parameters. Assume that $b_1,\ldots,b_{k+1}$ are independently and that $\sigma_i^2 > 0$ (i=1,...,k) and $\sigma_{k+1}^2 > 0$. Define $\sigma^2 = (\sigma_1^2, \ldots, \sigma_k^2, \sigma_{k+1}^2)^T$, $\gamma_i = \sigma_i^2/\sigma_{k+1}^2$ (i = 1,...,k) and $\gamma = (\gamma_1,\ldots,\gamma_k)^T$.

We devise an exact 100 (1-α)% confidence region for the vector σ^2 of variance components. Essentially the same approach can be used to obtain an exact 100 (1-α)% confidence region for the vector γ of variance ratios. Confidence regions for σ^2 and γ can be of direct interest. They can also be used to obtain (generally conservative) confidence intervals for functions of σ^2 or γ (Spjotvoll, 1972; Khuri, 1981) and for linear combinations of the fixed and random effects, that is, linear combinations of the elements of the vectors β_0, b_1, ..., b_k (Jeske, 1985).

Let $\chi^2(f)$ represent a chi-square distribution with f degrees of freedom, and take $\chi_{\alpha,f}^*$ to be the upper-α point of this distribution. Under certain circumstances, there exist k+1 quadratic forms

$y^T A_1 y, \ldots, y^T A_{k+1} y$, where $A_1, \ldots, A_{k+1}$ are $n \times n$ symmetric matrices of known constants, such that (i) $y^T A_1 y, \ldots, y^T A_{k+1} y$ are distributed independently, (ii) $y^T A_i y / (\sigma_{k+1}^2 c_i) \sim \chi^2(f_i)$ for a positive integer f_i and a scalar c_i that are necessarily given by $f_i = \text{rank}(A_i)$ and and $c_i = f_i^{-1}(d_{i,k+1} + \Sigma_j d_{ij} \gamma_j)$ with $d_{ij} = \text{tr}(X_j^T A_i X_j)$ ($j=1,\ldots,k$) and $d_{i,k+1} = \text{tr}(A_i)$ ($i=1,\ldots,k+1$), and (iii) the $(k+1) \times (k+1)$ matrix with ijth element d_{ij} is nonsingular. If the $k+1$ quadratic forms $y^T A_1 y, \ldots,$ $y^T A_{k+1} y$ exist, then clearly, for $0 < \alpha < 1$, a $100 (1-\alpha)\%$ confidence region for the vector σ^2 is given by the set $S(y)$ consisting of those values of the vector σ^2 that simultaneously satisfy the $k+1$ inequalities

$$(1.2) \qquad \chi^*_{1-\alpha_{i2}, f_i} < y^T A_i y / (\sigma_{k+1}^2 c_i) < \chi^*_{\alpha_{i1}, f_i} \quad (i=1,\ldots,k+1),$$

where α_{i1} and α_{i2} represent nonnegative constants such that $\alpha_{i1} + \alpha_{i2} < 1$ ($i=1,\ldots,k+1$) and $\Pi_i(1-\alpha_{i1}- \alpha_{i2}) = 1-\alpha$.

It is well known that, for balanced classificatory models, the requisite quadratic forms exist and, in fact, can be taken to be those sums of squares in the customary analysis of variance that correspond to the random effects and errors, in which case $f_1 + \ldots + f_k = n - \text{rank}(X_0)$ (e.g., Broemeling, 1969). Other special cases for which such quadratic forms have been found are treated by, for example, Broemeling and Bee (1976).

Unfortunately, in many cases, quadratic forms $y^T A_1 y, \ldots, y^T A_{k+1} y$, whose matrices $A_1, \ldots, A_{k+1}$ are matrices of known constants and that satisfy the three desired conditions, may, if they exist at all, be hard to find and/or may be such that $\Sigma f_i < n - \text{rank}(X_0)$, in which case the confidence region $S(y)$ may be overly large. In what follows, we present a general procedure for forming an exact $100(1-\alpha)\%$ confidence region for the vector σ^2. Our approach differs from the aforementioned approach in that we allow the elements of the matrix A_i of the ith quadratic form $y^T A_i y$ to be functionally dependent on the last $k-i+1$ variance ratios $\gamma_1 = \sigma_1^2/\sigma_{k+1}^2, \ldots, \gamma_k = \sigma_k^2/\sigma_{k+1}^2$ $(i=1,\ldots,k)$. By allowing this dependence, we are able to construct quadratic forms $y^T A_1 y, \ldots, y^T A_{k+1} y$ that satisfy the three desired properties and which, in addition, are such that $\Sigma f_i = n - \text{rank}(X_0)$. Then, as in the aforementioned approach, an exact $100(1-\alpha)\%$ confidence region consists of the set $S(y)$ of all values of the vector σ^2 that simultaneously satisfy the k+1 inequalities (1.2).

Our procedure can be regarded as an extension of Wald's (1940 and 1947) procedure. Wald's procedure, when extended along the lines discussed by Thompson (1955), Spjotvoll (1968), Seely and El-Bassiouni (1983), and Harville and Fenech (1984), covers the special case k=1. Hartley and Rao (1967, Sec. 9) proposed a general procedure for obtaining an exact $100(1-\alpha)\%$ confidence region which, like ours, can be viewed as a generalization of Wald's procedure. However, as can easily be shown, it produces confidence regions of a seemingly unappealing form and, in fact, can with high probability produce confidence regions of infinite volume.

In principle, the likelihood ratio could be used to generate a confidence region (Hartley and Rao, 1967, Sec. 8). However, the percentiles of its distribution are approximated on the basis of asymptotic results. The accuracy of these approximations is questionable and is not easily investigated. (What few asymptotic results are available for mixed linear models—see, for example, Miller (1977)—seem unassuring, and, except in special cases, Monte Carlo studies are computationally unfeasible.)

2. PRELIMINARIES

Define $V_i = I + \Sigma_{s=i+1}^{k}\gamma_s X_s X_s^T$ $(i=0,\ldots,k-1)$ and $V_{k+1} = V_k = I$, and let $V = V_0 = I + \Sigma_{s=1}^{k}\gamma_s X_s X_s^T$. Under the assumed model (1.1), $y \sim N(X_0\beta_0, \sigma_{k+1}^2 V)$, and the parameter space for the vector σ^2 is

$$\Omega_0 = \left\{\sigma^2 : \sigma_{k+1}^2 > 0, \gamma_i > 0 \ (i=1,\ldots,k)\right\}.$$

Note, however, that the matrix V is positive definite for some values of the vector γ that include one or more negative elements.

Subsequently, we take the model to be the generalization of model (1.1) that results from disregarding our original definitions of $\sigma_1^2,\ldots,\sigma_{k+1}^2$ as variances and from assuming only that $y \sim N(X_0\beta_0, \sigma_{k+1}^2 V)$ and that the parameter space for the vector σ^2 is

$$\Omega = \left\{\sigma^2 : \sigma_{k+1}^2 > 0, (\gamma_{i+1},\ldots,\gamma_k)^T \in \Gamma_i \ (i=0,\ldots,k-1)\right\},$$

where Γ_i is the set of all values of $(\gamma_{i+1}, \ldots, \gamma_k)^T$ such that V_i is positive definite.

We shall have occasion to refer to a model, to be called Model i, in which

$$y = X_0 \beta_0 + X_1 \beta_1 + \ldots + X_i \beta_i + e_i,$$

where $\beta_1, \ldots, \beta_i$ are vectors which, like β_0, are composed of unknown parameters, where e_i is an n x 1 unobservable random vector with $E(e_i) = 0$ and $var(e_i) = \sigma^2_{k+1} V_i$, and where $\gamma_{i+1}, \ldots, \gamma_k$ and hence V_i are assumed to be known $(i=1, \ldots, k)$. Model i is essentially the same as model (1.1) except that the parameter vectors $\beta_1, \ldots, \beta_i$ appear in place of the random vectors $b_1, \ldots, b_i$ and the parameters $\gamma_{i+1}, \ldots, \gamma_k$ are taken to be known instead of unknown.

For $i = 0, 1, \ldots, k$, define $X_i^* = (X_0, X_1, \ldots, X_i)$. Note that $X_i^* = (X_{i-1}^*, X_i)$ $(i=1, \ldots, k)$. Let $r_0 = rank(X_0)$, $r_i = rank(X_i^*) - rank(X_{i-1}^*)$ $(i=1, \ldots, k)$, and $r_{k+1} = n - rank(X_k^*)$. Subsequently, we assume that $r_i > 0$ $(i=1, \ldots, k+1)$.

We write A^- for an arbitrary generalized inverse of a matrix A, that is, A^- is any matrix satisfying $AA^-A = A$. Define

$$P_{i-1} = X_{i-1}^* (X_{i-1}^{*T} V_i^{-1} X_{i-1}^*)^- X_{i-1}^{*T} V_i^{-1} \qquad (i=1, \ldots, k+1).$$

Note that

$$P_{i-1}^2 = P_{i-1}, \quad P_{i-1}^T V_i^{-1} = (V_i^{-1} P_{i-1})^T = V_i^{-1} P_{i-1}$$

and that $P_{i-1} X_{i-1}^* = X_{i-1}^*$ and $X_{i-1}^{*T} V_i^{-1} P_{i-1} = (P_{i-1} X_{i-1}^*)^T V_i^{-1} = X_{i-1}^{*T} V_i^{-1}$,

implying that, for $j = 0, \ldots, i-1$,

$$P_{i-1}X_j = X_j, \quad X_j^T V_i^{-1} P_{i-1} = X_j^T V_i^{-1}, \quad P_{i-1}X_j^* = X_j^*, \quad X_j^{*T} V_i^{-1} P_{i-1} = X_j^{*T} V_i^{-1}$$

$(i=1,\ldots,k+1)$. Note also that, since the matrix $I-P_k = I - X_k^*(X_k^{*T}X_k^*)^- X_k^*$ is symmetric and idempotent, there exists an $n \times r_{k+1}$ matrix F such that $I-P_k = FF^T$ and $F^T F = I$ and that $FF^T X_i = 0$, implying that $F^T X_i = 0$ $(i=0,\ldots,k)$.

3. QUADRATIC FORMS

3.1 Definition

We now introduce the quadratic forms on which the proposed confidence region is to be based.

Define $C_i = X_i^T V_i^{-1}(I-P_{i-1})X_i$ and $q_i = X_i^T V_i^{-1}(I-P_{i-1})y$ $(i=1,\ldots,k)$. It is known that rank $(C_i) = r_i$ and that there exists an $m_i \times r_i$ matrix Λ_i of rank r_i such that, under Model i, $\tau_i = \Lambda_i^T \beta_i$ would be an estimable parametric function. It is further known that $\Lambda_i^T = L_i^T C_i$ for some matrix L_i, which is necessarily of rank r_i, and that, under Model i, the minimum-variance linear unbiased estimator of τ_i would be

$$\tilde{\tau}_i = (\tilde{\tau}_{i1}, \ldots, \tilde{\tau}_{ir_i})^T = L_i^T q_i.$$

The proposed confidence region is based on the $k+1$ quadratic forms

$$Q_i = Q_i(\gamma_1, \ldots, \gamma_k; y) = \tilde{\tau}_i^T [L_i^T(C_i + \gamma_i C_i^2)L_i]^{-1}\tilde{\tau}_i \quad (i=1,\ldots,k),$$

$$Q_{k+1} = Q_{k+1}(y) = y^T(I-P_k)y = z^T z,$$

where $z = F^T y$. As shown in Section 3.2, $Q_1/\sigma^2_{k+1}, \ldots, Q_{k+1}/\sigma^2_{k+1}$ are distributed independently as chi-square random variables with degrees of freedom $r_1, \ldots, r_{k+1}$, respectively. The quadratic forms $Q_1, \ldots, Q_{k+1}$ are invariant to the choice of the matrices $\Lambda_1, \ldots, \Lambda_k$, as is easily verified.

3.2 Joint distribution

Under the assumed distribution for y, which is $N(X_0 \beta_0, \sigma^2_{k+1} V)$, we find that, for $j < i = 1, \ldots, k$, $cov(q_i, q_j)$

$$= \sigma^2_{k+1} X_i^T V_i^{-1} (I - P_{i-1}) V V_j^{-1} (I - P_{j-1}) X_j$$

$$= \sigma^2_{k+1} X_i^T V_i^{-1} (I - P_{i-1})(I + \Sigma^k_{s=j} \gamma_s X_s X_s^T) V_j^{-1} (I - P_{j-1}) X_j$$

$$= \sigma^2_{k+1} X_i^T V_i^{-1} (I - P_{i-1})(V_j + \gamma_j X_j X_j^T) V_j^{-1} (I - P_{j-1}) X_j$$

$$= \sigma^2_{k+1} X_i^T V_i^{-1} (I - P_{i-1}) V_j V_j^{-1} (I - P_{j-1}) X_j$$

$$= \sigma^2_{k+1} [X_i^T V_i^{-1} (I - P_{i-1}) X_j - X_i^T V_i^{-1} (I - P_{i-1}) X^*_{j-1} (X^{*T}_{j-1} V_j^{-1} X^*_{j-1})^- X^{*T}_{j-1} V_j^{-1} X_j]$$

(3.1) $$= 0 - 0 = 0.$$

It can be shown, in similar fashion, that $cov(z, q_j) = 0$ $(j=1, \ldots, k)$. Thus, $q_1, \ldots, q_k, z$ are distributed independently, implying that $\tilde{\tau}_1, \ldots, \tilde{\tau}_k, z$ are distributed independently and hence that $Q_1, \ldots, Q_k, Q_{k+1}$ are distributed independently.

Further, for $i=1,\ldots,k$, we find that

$$(3.2) \qquad E(q_i) = X_i^T V_i^{-1}(I-P_{i-1})X_0\beta_0 = 0,$$

$$var(q_i) = \sigma_{k+1}^2 X_i^T V_i^{-1}(I-P_{i-1})VV_i^{-1}(I-P_{i-1})X_i$$

$$= \sigma_{k+1}^2 X_i^T V_i^{-1}(I-P_{i-1})(V_i + \gamma_i X_i X_i^T)V_i^{-1}(I-P_{i-1})X_i$$

$$(3.3) \qquad = \sigma_{k+1}^2(C_i + \gamma_i C_i^2),$$

implying that $\tilde{\tau}_i \sim N[0, \sigma_{k+1}^2 L_i^T(C_i + \gamma_i C_i^2)L_i]$ and hence that $Q_i/\sigma_{k+1}^2 \sim \chi^2(r_i)$. Also, $z \sim N(0,\sigma_{k+1}^2 I)$, and, consequently, $Q_{k+1}/\sigma_{k+1}^2 \sim \chi^2(r_{k+1})$.

3.3 Canonical representation

We now consider a particular choice for the parameter vectors $\tau_1,\ldots,\tau_k$ or, equivalently, for the coefficient matrices $\Lambda_1^T,\ldots,\Lambda_k^T$. This choice produces representations for the quadratic forms $Q_1,\ldots,Q_k$ that are, as we discuss in Section 4, informative about the nature of the proposed confidence region, and that can be useful computationally.

Let $\Delta_{i1},\ldots,\Delta_{ir_i}$ represent the nonzero, and hence positive, characteristic values of the matrix C_i, define $D_i = diag(\Delta_{i1},\ldots,\Delta_{ir_i})$, and take R_i to be an $m_i \times r_i$ matrix whose columns are orthonormal characteristic vectors of C_i corresponding to the values $\Delta_{i1},\ldots,\Delta_{ir_i}$,

respectively. Thus, by definition,

$$C_1 R_1 = R_1 D_1, \qquad R_1^T R_1 = I,$$

implying that

$$R_1^T C_1 R_1 = D_1, \qquad R_1^T C_1^2 R_1 = (C_1 R_1)^T C_1 R_1 = D_1 R_1^T R_1 D_1 = D_1^2.$$

Consider the choice

$$\Lambda_1^T = D_1^{-1/2} R_1^T C_1 = L_1^T C_1$$

with $L_1^T = D_1^{-1/2} R_1^T$. Note that this choice varies with $\gamma_{i+1}, \ldots, \gamma_k$. It

leads to the representation

$$(3.4) \qquad Q_1 = \tilde{\tau}_1^T (I + \gamma_1 D_1)^{-1} \tilde{\tau}_1 = \sum_{j=1}^{r_1} \frac{\tilde{\tau}_{1j}^2}{1 + \gamma_1 \Delta_{1j}}$$

with $\tilde{\tau}_1 = D_1^{-1/2} R_1^T q_1$.

3.4 An alternative approach

The quadratic forms $Q_1, \ldots, Q_{k+1}$ can be defined, and their

properties established, via a vector-space approach, as we now

demonstrate. Denote by R^n the vector space consisting of all

n-dimensional real vectors, and let $W^\perp$ represent the orthogonal

complement of a subspace W of R^n with respect to the usual inner product,

that is, the inner product that assigns the value $y_1^T y_2$ to any two

n-dimensional real vectors y_1 and y_2. Further, let $W^{\perp i}$ represent the

orthogonal complement of W with respect to the inner product $y_1^T V_1 y_2$.

Denote by C(A) the column space of a matrix A.

Define $U_{k+1} = C(X_k^*)^\perp$ and

$$U_i = C(X_{i-1}^*)^\perp \cap [C(X_i^*)^\perp]^{\perp_i} \qquad (i=1,\dots,k).$$

Then, $\dim(U_{k+1}) = r_{k+1}$ and

$$\dim(U_i) = \dim[C(X_{i-1}^*)^\perp] - \dim[C(X_i^*)^\perp]$$

$$= n - \mathrm{rank}(X_{i-1}^*) - [n - \mathrm{rank}(X_i^*)] = r_i \qquad (i=1,\dots,k).$$

Take H_i to be an $n \times r_i$ matrix whose columns form a basis for U_i $(i=1,\dots,k+1)$. Derivations paralleling those of results (3.1), (3.2), and (3.3) reveal that $H_i^T V H_j = 0$ $(j<i=1,\dots,k+1)$, that $H_i^T X_0 = 0$ $(i=1,\dots,k+1)$, and that $H_i^T V H_i = H_i^T (V_i + \gamma_i X_i X_i^T) H_i$ $(i=1,\dots,k)$ and $H_{k+1}^T V H_{k+1} = H_{k+1}^T H_{k+1}$. Note that $U_1,\dots,U_{k+1}$ are orthogonal with respect to the inner product $y_1^T V y_2$ and that their direct sum is $C(X_0)^\perp$.

We have, in effect, established that the vectors $H_1^T y,\dots,H_{k+1}^T y$ are distributed independently, with $H_i^T y \sim N[0, \sigma_{k+1}^2 H_i^T (V_i + \gamma_i X_i X_i^T) H_i]$ $(i=1,\dots,k)$ and $H_{k+1}^T y \sim N(0, \sigma_{k+1}^2 H_{k+1}^T H_{k+1})$. It follows that the $k+1$ quadratic forms

$$Q_i^* = y^T H_i [H_i^T (V_i + \gamma_i X_i X_i^T) H_i]^{-1} H_i^T y \qquad (i=1,\dots,k)$$

$$Q_{k+1}^* = y^T H_{k+1} (H_{k+1}^T H_{k+1})^{-1} H_{k+1}^T y$$

are distributed independently, with $Q_i^*/\sigma_{k+1}^2 \sim \chi^2(r_i)$ $(i=1,\dots,k+1)$. These quadratic forms are invariant to the choice of the basis matrices $H_1,\dots,H_{k+1}$, as is easily verified.

It is easy to show that one choice for the matrices $H_1^T, \ldots, H_{k+1}^T$ is $H_i^T = L_i^T X_i^T V_i^{-1}(I-P_{i-1})$ $(i=1,\ldots,k)$, $H_{k+1}^T = F^T$. This result can, in turn, be used to show that the quadratic forms $Q_1^*, \ldots, Q_{k+1}^*$ are identical to the quadratic forms $Q_1, \ldots, Q_{k+1}$, introduced in Section 3.1. The representations $Q_1, \ldots, Q_{k+1}$ are informative about the nature of the computations required to evaluate the k+1 quadratic forms for specified values of $\gamma_1, \ldots, \gamma_k$.

4. NATURE OF CONFIDENCE REGION

4.1 General case

The set $S(y)$, consisting of those values of the vector σ^2 ($\sigma^2 \in \Omega$) that simultaneously satisfy the k+1 inequalities

$$\chi_{1-\alpha_{i2}, r_i}^* < Q_i/\sigma_{k+1}^2 < \chi_{\alpha_{i1}, r_i}^* \quad (i=1,\ldots,k+1),$$

is a $100(1-\alpha)\%$ confidence region for σ^2. We now present an alternative description of this set, one which provides more insight into the nature of the set and which is more useful computationally.

Let λ_i^* represent the maximum characteristic value of the matrix $X_i^T V_i^{-1} X_i$, and define $\Delta_i^* = \max(\Delta_{i1}, \ldots, \Delta_{ir_i})$ $(i=1,\ldots,k)$. It is easy to show that $\Delta_i^* < \lambda_i^*$. For any fixed value of $(\gamma_{i+1}, \ldots, \gamma_k) \in \Gamma_i$, the matrix $V_{i-1} = V_i + \gamma_i X_i X_i^T$ is positive definite for those values of γ_i belonging to the interval $-1/\lambda_i^* < \gamma_i < \infty$, but the quadratic form Q_i is a well-defined function of γ_i over the more extensive interval $-1/\Delta_i^* < \gamma_i < \infty$, as is evident from representation (3.4). Further, as a function of γ_i, Q_i is

strictly decreasing and strictly convex over the interval $-1/\Delta_i^* < \gamma_i < \infty$, and

$$\underset{\gamma_i \to -1/\Delta_i^*}{\text{limit}} Q_i = \infty, \qquad \underset{\gamma_i \to \infty}{\text{limit}} Q_i = 0$$

(Harville and Fenech, 1984, Section 3). For convenience, define

$Q_i(-1/\Delta_i^*, \gamma_{i+1},\ldots,\gamma_k;y) = \infty$ and $Q_i(\infty,\gamma_{i+1},\ldots,\gamma_k;y) = 0$.

Let $\ell_{k+1} = \ell_{k+1}(y) = Q_{k+1}/\chi^{*2}_{\alpha_{k+1,1},r_{k+1}}$ and $u_{k+1} = u_{k+1}(y) = Q_{k+1}/\chi^{*2}_{1-\alpha_{k+1,2},r_{k+1}}$. Further, for any fixed value of $(\gamma_{i+1},\ldots,\gamma_k) \in \Gamma_i$ and for any fixed positive value of σ^2_{k+1}, define $\ell_i = \ell_i(\gamma_{i+1},\ldots,\gamma_k, \sigma^2_{k+1};y)$ to be the unique value of γ_i that satisfies $Q_i = \sigma^2_{k+1}\chi^{*2}_{\alpha_{i1},r_i}$ and $u_i = u_i(\gamma_{i+1},\ldots,\gamma_k,\sigma^2_{k+1};y)$ to be the unique value of γ_i that satisfies $Q_i = \sigma^2_{k+1}\chi^{*2}_{1-\alpha_{i2},r_i}$. Then, an alternative description of the $100(1-\alpha)\%$ confidence region $S(y)$ is $S(y) =$

$$\{\sigma^2 : \sigma^2 \in \Omega, \ell_{k+1} < \sigma^2_{k+1} < u_{k+1}, \sigma^2_{k+1}\ell_i < \sigma^2_i < \sigma^2_{k+1}u_i \ (i=1,\ldots,k)\}.$$

4.2 Special case

The upper and lower bounds u_i and ℓ_i on γ_i were defined as solutions to equations in γ_i which are, in general, inherently nonlinear and not amenable to explicit solution. We now consider a special case where these equations can be solved explicitly.

Let $P^{(0)}_{i-1}$ represent the value of the matrix P_{i-1} when $\gamma_{i+1} = \ldots = \gamma_k = 0$; that is, $P^{(0)}_{i-1} = X^*_{i-1}(X^{*T}_{i-1}X^*_{i-1})^- X^*_{i-1} (i=1,\ldots,k+1)$. Note that the quadratic form $y^T(I-P^{(0)}_0)y$ represents the residual sum of squares obtained from a least squares fit of the submodel $y = X_0\beta_0 + b_{k+1}$.

Following Brown (1984), we define an <u>analysis of variance for the</u>

<u>variance components</u> to be a partitioning $y^T(I-P_0^{(0)})y = y^TA_1y + \ldots + y^TA_sy$,

where $A_1,\ldots,A_s$ are n x n symmetric matrices of known constants, such that

(i) $y^TA_1y,\ldots,y^TA_sy$ are distributed independently, (ii) $y^TA_iy/(\sigma_{k+1}^2c_i) \sim$

$\chi^2(f_i)$ for a positive integer f_i and a scalar c_i (i=1,...,s), and (iii)

the scalars $c_1,\ldots,c_s$, which are necessarily linear functions of $\gamma_1,\ldots,\gamma_k$,

are distinct. Brown showed, in effect, that an analysis of variance for

the variance components exists if and only if the matrices

$(I-P_0^{(0)})X_1X_1^T(I-P_0^{(0)}),\ldots,(I-P_0^{(0)})X_kX_k^T(I-P_0^{(0)})$ commute in pairs, in which

case the sums of squares $y^TA_1y,\ldots,y^TA_sy$ are unique up to order.

In the Appendix, we show, by construction, that, if an analysis of

variance for the variance components exists, then

$$Q_i = \Sigma_{j\epsilon I_i}y^TA_jy/c_j \qquad (i=1,\ldots,k+1),$$

where $I_1,\ldots,I_{k+1}$ represents a partitioning of the integers $1,\ldots,s$ into

k+1 sets. We show further that, if s = k+1, then, for i=1,...,k,

$$Q_i = \frac{y^T(P_i^{(0)} - P_{i-1}^{(0)})y}{1 + \Sigma_{j=i}^k\lambda_{ji}\gamma_j}$$

where $\lambda_{ji} = r_i^{-1}tr[X_j^T(P_i^{(0)} - P_{i-1}^{(0)})X_j]$ (j=1,...,k).

We see that, in the special case where there exists an analysis of

variance for the variance components and where, in addition, s = k+1,

(4.1) $\ell_i = \lambda_{ii}^{-1}[y^T(P_i^{(0)}-P_{i-1}^{(0)})y/(\sigma_{k+1}^2\chi_{\alpha_{ii},r_i}^*) - (1 + \Sigma_{j=i+1}^k\lambda_{ji}\gamma_j)]$,

(4.2) $u_i = \lambda_{11}^{-1}[y^T(P_i^{(0)}-P_{i-1}^{(0)})y/(\sigma_{k+1}^2\chi^{*}_{1-\alpha_{12},r_i}) - (1 + \Sigma_{j=i+1}^k\lambda_{ji}\gamma_j)]$,

and that, for balanced classificatory models, our procedure for forming a confidence region reduces to the traditional procedure. Note that, in this special case, ℓ_i and u_i are linear functions of $\gamma_{i+1},\ldots,\gamma_k$ and $1/\sigma_{k+1}^2$ or, equivalently, $\sigma_{k+1}^2\ell_i$ and $\sigma_{k+1}^2u_i$ are linear functions of $\sigma_{i+1}^2,\ldots,\sigma_k^2$, σ_{k+1}^2.

Even if an analysis of variance for all k+1 variance components does not exist, there may exist a less extensive partitioning $y^T(I-P_{k'}^{(0)})y = y^TA_1y + \ldots + y^TA_sy$ such that $y^TA_1y,\ldots,y^TA_sy$ are distributed independently as distinct scalar multiples of chi-square random variables, in which case formulas (4.1) and (4.2) are still applicable, at least for $i = k'+1,\ldots,k$.

5. DISCUSSION

Some modifications of the proposed procedure for obtaining a confidence region for the variance components $\sigma_1^2,\ldots,\sigma_{k+1}^2$ and some considerations in its implementation are as follows:

1. The proposed procedure can be modified so as to obtain a confidence region for the variance ratios $\gamma_1,\ldots,\gamma_k$. Define $F_i = (r_{k+1}/r_i)(\chi_i^2/\chi_{k+1}^2)$ $(i=1,\ldots,k)$, where $\chi_1^2,\ldots,\chi_{k+1}^2$ represent independently distributed chi-square random variables with degrees of freedom $r_1,\ldots,r_{k+1}$, respectively. Take $F_i^{(\ell)}$, $F_i^{(u)}$ $(i=1,\ldots,k)$ to be any constants such that

$$pr[F_i^{(\ell)} < F_i < F_i^{(u)} \; (i=1,\ldots,k)] = 1-\alpha.$$

Then, a 100(1-α)% confidence region for $\gamma_1,\ldots,\gamma_k$ is the set

$$s^{*}(y) = \{\gamma : (\gamma_1,\ldots,\gamma_k)^T \epsilon \Gamma_{i-1}, \; \ell_i^{*} < \gamma_i < u_i^{*} \; (i=1,\ldots,k)\}$$

where $\ell_i^* = \ell_i^*(\gamma_{i+1},\ldots,\gamma_k;y)$ is the unique value of γ_i that satisfies $(r_{k+1}/r_i)(Q_i/Q_{k+1}) = F_i^{(u)}$ and $u_i^* = u_i^*(\gamma_{i+1},\ldots,\gamma_k;y)$ is the unique value of γ_i that satisfies $(r_{k+1}/r_i)(Q_i/Q_{k+1}) = F_i^{(\ell)}$. In the special case of a balanced classificatory model and for $\alpha_{11} = \ldots = \alpha_{k1} = 0$, the confidence region $S^*(y)$ simplifies to that discussed by Sahai and Anderson (1973).

If k is sufficiently large, the determination of the constants $F_i^{(\ell)}$, $F_i^{(u)}$ ($i=1,\ldots,k$) may be computationally unfeasible, in which case our procedure for obtaining an exact $100(1-\alpha)\%$ confidence region can not be implemented. However, an approximate $100(1-\alpha)\%$ confidence region can be obtained by replacing $F_i^{(\ell)}$ and $F_i^{(u)}$ by the upper-$(1-\alpha_{i2})$ and upper-α_{i1} points, respectively, of the marginal distribution of F_i. It follows from Kimball's (1951) inequality that, for $\alpha_{12} = \ldots = \alpha_{k2} = 0$, this region is conservative; that is, its probability of coverage equals or exceeds $1-\alpha$. In the special case of a balanced classificatory model and for $\alpha_{11} = \ldots = \alpha_{k1} = 0$, the approximate confidence region simplifies to that proposed by Broemeling (1969).

2. The proposed procedure for using the quantities $Q_1,\ldots,Q_{k+1}$ to form a confidence region for the variance components $\sigma_1^2,\ldots,\sigma_{k+1}^2$ or the variance ratios $\gamma_1,\ldots,\gamma_k$ can be modified, in an obvious way, to obtain a confidence region for the last $k-k^*+2$ variance components $\sigma_{k^*}^2,\ldots,\sigma_{k+1}^2$ or the last $k-k^*+1$ variance ratios $\gamma_{k^*},\ldots,\gamma_k$, based on the quantities $Q_{k^*},\ldots,Q_{k+1}$.

3. By following the approach described, for example, by Spjotvoll (1972) and Khuri (1981), the proposed confidence region for the variance components $\sigma_1^2,\ldots,\sigma_{k+1}^2$ or variance ratios $\gamma_1,\ldots,\gamma_k$ can be transformed into a generally conservative confidence region for a function of the variance components or variance ratios or, more generally, for a family of such functions. For instance, let $R_f(y)$ represent the range of a vector $f = f(\sigma_1^2,\ldots,\sigma_{k+1}^2)$ of functions of variance components when the domain of f is restricted to the set $S(y)$. Then, clearly, $pr[f \epsilon R_f(y)] > 1-\alpha$; that is, $R_f(y)$ is a generally conservative $100(1-\alpha)\%$ confidence region for f.

4. Often, the parameter space for the vector σ^2 is a proper subset Ω' of the set Ω, rather than Ω itself. In particular, the parameter space for σ^2 may be the set Ω_0.

The confidence region $S(y)$ may include values of σ^2 not belonging to Ω'. Let $S'(y)$ represent the subset of $S(y)$ obtained by deleting all such values. For $\sigma^2 \epsilon \Omega'$, $pr[\sigma^2 \epsilon S'(y)] = pr[\sigma^2 \epsilon S(y)] = 1-\alpha$. Thus, when the parameter space for σ^2 is Ω', $S'(y)$, like $S(y)$, is a $100(1-\alpha)\%$ confidence region for σ^2.

In the special case $\Omega' = \Omega_0$, the $100(1-\alpha)\%$ confidence region $S'(y)$ is obtained from $S(y)$ by deleting all values of σ^2 for which one or more of the first k variance components $\sigma_1^2,\ldots,\sigma_k^2$ is negative. Expanding the set $S'(y)$ slightly, we obtain the set $S^+(y) = \{\sigma^2: \sigma_{k+1}^2 > 0, \ell_{k+1}<\sigma_{k+1}^2<u_{k+1}, \sigma_{k+1}^2 \max(\ell_1,0)<\sigma_1^2<\sigma_{k+1}^2 \max(u_1,0) \ (i=1,\ldots,k)\}$.
We have that $pr[\sigma^2 \epsilon S^+(y)]$ equals $1-\alpha$, if $\sigma_1^2 > 0$ for $i=1,\ldots,k$, and is

greater than or equal to $1-\alpha$, otherwise, as is easily verified. Thus, when the parameter space for σ^2 is Ω_0, $S^+(y)$ is a conservative $100(1-\alpha)\%$ confidence region. Unlike $S'(y)$, the set $S^+(y)$ is nonempty, with probability one.

5. There will generally be more than one way to express a particular mixed or random linear model as a special case of the general mixed linear model (1.1). Consider, for example, the customary additive model for a two-way crossed classification with both factors regarded as random. We can take the elements of b_1 to be the effects of the first factor or, alternatively, the effects of the second factor.

It should be noted that, except for highly structured situations, like those considered in Section 4.2, the confidence region $S(y)$ will vary with the order in which we assign the various sets of random effects to the vectors $b_1, \ldots, b_k$.

6. Note that, by exploiting general relationships between confidence regions and tests of hypothesis or significance, the proposed procedure for forming a confidence region can be used to test, against appropriate alternatives, a null hypothesis of the general form $H_o: \sigma_1^2 = c_1, \ldots, \sigma_{k+1}^2 = c_{k+1}$ or $H_o: \gamma_1 = c_1, \ldots, \gamma_k = c_k$, where $c_1, \ldots, c_{k+1}$ represent specified constants.

Also, following Harville and Fenech (1984, Section 7), we can obtain point estimators of the variance components or variance ratios by equating the pivotal quantities $Q_1/\sigma_{k+1}^2, \ldots, Q_{k+1}/\sigma_{k+1}^2$ or $(r_{k+1}/r_1)Q_1/Q_{k+1}, \ldots, (r_{k+1}/r_k)Q_k/Q_{k+1}$ to appropriately chosen constants. In

particular, if we equate $Q_1/\sigma^2_{k+1},\ldots,Q_{k+1}/\sigma^2_{k+1}$ to $r_1,\ldots,r_{k+1}$,
respectively, we obtain estimators which, in the special case where
there exists an analysis of variance for the variance components and
where $s = k+1$, simplify to the usual analysis-of-variance estimators.
Alternatively, if we equate these quantities to the medians of their
respective chi-square distributions, we obtain estimators that can
be interpreted as the coordinates of a degenerate, single-point
confidence region.

7.   Let $Q_. = Q_1 + \ldots + Q_k$ and $r_. = r_1 + \ldots + r_k$, and define $F^{(\ell)}$ and
$F^{(u)}$ to be any constants such that $\text{pr}[F^{(\ell)} < F < F^{(u)}] = 1-\alpha$, where F
represents an F random variable with degrees of freedom $r_.$ and r_{k+1},
respectively. Clearly, the distribution of $Q_./\sigma^2_{k+1}$ is $\chi^2(r_.)$, and $Q_.$ and
Q_{k+1} are distributed independently. It follows that an exact $100(1-\alpha)\%$
confidence region for $\gamma_1,\ldots,\gamma_k$, alternative to the confidence region
$S^*(y)$, is the set $S^\#(y)$ consisting of those values of γ that satisfy the
inequality

$$F^{(\ell)} < (r_{k+1}/r_k)Q_./Q_{k+1} < F^{(u)}.$$

It can be shown that, in the special case where $F^{(\ell)} = 0$ (and hence
where $F^{(u)}$ is the upper-α point of the distribution of F), the confidence
region $S^\#(y)$ is the same as the exact confidence region devised by Hartley
and Rao (1967, Sec. 9). We do not recommend the confidence region $S^\#(y)$

since, as previously indicated in the special case of the Hartley-Rao

region, it has a seemingly unappealing form and can, with high

probability, produce confidence regions of infinite volume.

8. In practice, we may want to display graphically the confidence

region $S(y)$, or when k exceeds one or two, to display, for each of various

fixed values of the vector $(\sigma_{i+1}^2,\ldots,\sigma_k^2, \sigma_{k+1}^2)$ and the integer i, the

interval of σ_i^2 values, or perhaps the two- or three-dimensional set of

σ_{i-1}^2, σ_i^2 or σ_{i-2}^2, σ_{i-1}^2, σ_i^2 values, that are represented in $S(y)$. We are

then faced with the computational problem of determining the numerical

values of ℓ_i and u_i corresponding to each value of $(\sigma_{i+1}^2,\ldots,\sigma_k^2,\sigma_{k+1}^2)$

and each value of i.

In the special case where there exists an analysis of variance

for the variance components and where $s = k+1$, this problem reduces,

in effect, to that of computing the entries in the analysis-of-variance

table. More generally, we can use the approach discussed, in the

special case $i = k$, by Harville and Fenech (1984, Section 4), to compute

the values of $\Delta_{i1},\ldots,\Delta_{ir_i}$ and of $\Upsilon_{i1},\ldots,\Upsilon_{ir_i}$ and to then determine the

values of ℓ_i and u_i graphically or iteratively. How a series of such

determinations, involving various values of the vector $(\sigma_{i+1}^2,\ldots,\sigma_k^2,\sigma_{k+1}^2)$

and/or the integer i, might be accomplished most efficiently is a question

for possible investigation.

APPENDIX

Simplification of the quadratic forms

We now derive, for the special case where there exists an analysis of variance for the variance components, the simplified representations given in Section 4.2 for the quadratic forms $Q_1, \ldots, Q_k$.

Let $U_0^{(0)} = C(X_0)$, $U_i^{(0)} = C(X_{i-1}^*)^\perp \cap C(X_i^*)$ $(i=1,\ldots,k)$, and $U_{k+1}^{(0)} = C(X_k^*)^\perp$, so that, for $i=1,\ldots,k+1$, $U_i^{(0)}$ represents U_i when $\gamma_{i+1} = \ldots = \gamma_k = 0$. Define M_i to be an $n \times r_i$ matrix whose columns form an orthonormal basis for $U_i^{(0)}$ with respect to the ordinary inner product.

Note that the columns of the matrix $M_i^* = (M_0, \ldots, M_i)$ form an orthonormal basis for $C(X_i^*)$ $(i=0,\ldots,k)$ and that the columns of the matrix $M = (M_1, \ldots, M_{k+1})$ form an orthonormal basis for $C(X_0)^\perp$. Note also that, for $i=0,\ldots,k$,

$$M_i^* M_i^{*T} = M_i^* (M_i^{*T} M_i^*)^{-1} M_i^{*T} = X_i^* (X_i^{*T} X_i^*)^- X_i^{*T} = P_i^{(0)}$$

and that, for $i=1,\ldots,k$,

$$M_i M_i^T = M_i^* M_i^{*T} - M_{i-1}^* M_{i-1}^{*T} = P_i^{(0)} - P_{i-1}^{(0)},$$

$$X_i^T M_i M_i^T X_i = X_i^T (P_i^{(0)} - P_{i-1}^{(0)}) X_i = X_i^T (I - P_{i-1}^{(0)}) X_i,$$

(A.1) $\operatorname{rank}(M_i^T X_i X_i^T M_i) = \operatorname{rank}(X_i^T M_i M_i^T X_i) = \operatorname{rank}[X_i^T (I - P_{i-1}^{(0)}) X_i] = r_i.$

Suppose now that there exists an analysis of variance for the

variance components. Then, the k matrices $M^T X_i X_i^T M =$

$\text{diag}[(M_1, \ldots, M_i)^T X_i^T X_i (M_1, \ldots, M_i), 0]$ $(i=1, \ldots, k)$ commute in pairs

(Brown, 1984, Corollary 2), which implies that, for $i=1, \ldots, k$,

(A.2) $M_i^T X_i X_i^T M = \text{diag}(M_1^T X_i X_i^T M_1, \ldots, M_i^T X_i X_i^T M_i, 0, \ldots, 0)$,

as we now show.

Our proof of result (A.2) is by induction. The result is clearly

valid for $i=1$. Suppose that it is valid for $i=1, \ldots, i'-1$. Then, since

$M^T X_i X_i^T M$ and $M^T X_{i'} X_{i'}^T M$ commute, implying that the ijth block of the

matrix $M^T X_i X_i^T M M^T X_{i'} X_{i'}^T M$ is the same as that of $M^T X_{i'} X_{i'}^T M M^T X_i X_i^T M$,

we have, for $i=1, \ldots, i'-1$ and $j=i+1, \ldots, i'$, that

$$M_i^T X_i X_i^T M_i M_i^T X_{i'} X_{i'}^T M_j = 0$$

and hence, in light of result (A.1), that $M_i^T X_{i'} X_{i'}^T M_j = 0$. Observing that

$M^T X_i X_i^T M$ is symmetric, we conclude that result (A.2) is valid for $i=i'$,

which completes the proof of this result.

Now, since the matrices $M^T X_1 X_1^T M, \ldots, M^T X_k X_k^T M$ commute in pairs, we

have, in light of result (A.2), that the matrices $M_1^T X_1 X_1^T M_1, \ldots, M_1^T X_k X_k^T M_1$

commute in pairs. Consequently, there exists an orthogonal matrix that

simultaneously diagonalizes the matrices $M_1^T X_1 X_1^T M_1, \ldots, M_1^T X_k X_k^T M_1$; that is,

there exists an orthogonal matrix 0_1 such that

$$0_1^T M_1^T X_j X_j^T M_1 0_1 = \text{diag}(\lambda_{j11}, \ldots, \lambda_{j1r_1})$$

for some nonnegative real numbers $\lambda_{j11}, \ldots, \lambda_{j1r_1}$ $(j=1, \ldots, k)$.

As a further consequence of result (A.2), we have that

$$M_1^T V_1 (M_{i+1}, \ldots, M_{k+1}) = M_1^T (I + \Sigma_{s=i+1}^{k} \gamma_s X_s X_s^T)(M_{i+1}, \ldots, M_{k+1}) = 0,$$

implying that the columns of M_i, and hence those of $M_i O_i$, form a basis for U_i $(i=1, \ldots, k)$.

For $i=1, \ldots, k$, define

$$w_i = (w_{i1}, \ldots, w_{ir_i})^T = (M_i O_i)^T y,$$

define $c_{i1}, \ldots, c_{ir_i^*}$ to be the distinct linear functions represented among the r_i linear functions $1 + \Sigma_{j=1}^{k} \lambda_{ji1} \gamma_j, \ldots, 1 + \Sigma_{j=1}^{k} \lambda_{jir_i} \gamma_j$, and, for $m=1, \ldots, r_i^*$, take T_{im} to be the collection of values of the index t for which $1 + \Sigma_{j=1}^{k} \lambda_{jit} \gamma_j = c_{im}$, take f_{im} to be the dimension of this collection, and let $W_{im} = \Sigma_{t \epsilon T_{im}} w_{it}^2$.

It follows from the results of Section 3.4 that

$$Q_i = Q_i^* = y^T M_i O_i (I + \Sigma_{j=1}^{k} \gamma_j O_i^T M_i^T X_j X_j^T M_i O_i)^{-1} O_i^T M_i^T y$$

$$= \Sigma_{m=1}^{r_i^*} W_{im}/c_{im} \qquad (i=1, \ldots, k),$$

$$Q_{k+1} = Q_{k+1}^* = y^T M_{k+1} (M_{k+1}^T M_{k+1})^{-1} M_{k+1}^T y = y^T M_{k+1} M_{k+1}^T y.$$

Further we find that

$$\Sigma_{i=1}^{k} \Sigma_{m=1}^{r_i^*} W_{im} + Q_{k+1} = y^T M M^T y = y^T (I - M_0 M_0^T) y = y^T (I - P_0^{(0)}) y$$

and, proceeding as in Section 3.4, that $W_{im}(i=1, \ldots, k; m=1, \ldots, r_i^*)$, Q_{k+1} are distributed independently and $W_{im}/(c_{im} \sigma_{k+1}^2) \sim \chi^2(f_{im})$, implying that $W_{im}(i=1, \ldots, k; m=1, \ldots, r_i^*)$, Q_{k+1} are the sums of squares

in the analysis of variance for the variance components.

Now, suppose that the analysis of variance for the variance components is such that $s = k+1$. Then, for $i=1,\ldots,k$, $\lambda_{ji1} = \ldots = \lambda_{jir_i} = \lambda_{ji}$ for some real number λ_{ji} given by

$$\lambda_{ji} = r_i^{-1} \sum_{t=1}^{r_i} \lambda_{jit} = r_i^{-1} tr(0_i^T M_i^T X_j X_j^T M_i 0_i)$$

$$= r_i^{-1} tr(X_j^T M_i 0_i 0_i^T M_i^T X_j)$$

$$= r_i^{-1} tr[X_j^T (P_i^{(0)} - P_{i-1}^{(0)}) X_j] \quad (j=1,\ldots,k)$$

in which case

$$Q_i = w_i^T w_i / (1 + \sum_{j=1}^{k} \lambda_{ji} \gamma_j) = y^T M_i M_i^T y / (1 + \sum_{j=1}^{k} \lambda_{ji} \gamma_j)$$

$$= y^T (P_i^{(0)} - P_{i-1}^{(0)}) y / (1 + \sum_{j=1}^{k} \lambda_{ji} \gamma_j).$$

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We present a general procedure for obtaining exact confidence regions for the variance components in unbalanced mixed linear models. The procedure utilizes, as pivotal quantities, quadratic forms that may depend on the variance components in a complicated way and that are distributed independently as chi-square variates. In the special case of balanced classificatory models, the pivotal quantities simplify to scalar multiples of sums of squares from the usual analysis of variance. The procedure can be easily modified so as to obtain an exact confidence region for ratios

20. (continued)

of variance components and can be regarded as a generalization of Wald's procedure for obtaining a confidence interval for a single variance ratio.

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